

## Author index to volume 206

- Amorós, J., A prediction for the thermal conductivity coefficient of liquids along the saturation line 206 (1996) 301
- Andrés, J., see Moliner, V. 206 (1996) 57
- Arnau, A., see Moliner, V. 206 (1996) 57
- Baldwin, M.J., see Haydon, S.C. 206 (1996) 245
- Baumgarten, M., see Zhang, J. 206 (1996) 339
- Bauschlicher Jr., C.W., The structure of  $\text{Li}^-$  and  $\text{K}^-$  206 (1996) 35
- Bolton, K. and S. Nordholm, Classical trajectory study of collision induced intramolecular energy transfer in trans-stilbene 206 (1996) 103
- Chang, H.-C., see Wang, J.-H. 206 (1996) 43
- Chen, Y.-T., see Wang, J.-H. 206 (1996) 43
- Chou, K.-C., see Zhang, C.-T. 206 (1996) 271
- Costela, A. and I. Garcia-Moreno, Phase-conjugate reflection by degenerate four-wave mixing in 2-(2'-hydroxyphenyl)benzimidazole dye solutions: solvent effects 206 (1996) 383
- Crosley, D.R., see Luque, J. 206 (1996) 185
- De Almeida, W.B., see Resende, S.M. 206 (1996) 1
- Deng, C., see Wang, Y. 206 (1996) 279
- Dhuicq, D., O. Lehner, F. Linder and V. Sidis, Angular and energy analysis of  $\text{HeH}^+$  products from the charge exchange excitation reaction  $\text{He}^+ + \text{H}_2 \rightarrow \text{HeH}^+ + \text{H}^+$  206 (1996) 139
- Di Paolo, R.E. and J.O. Tocho, Polarization anisotropy applied to the determination of structural changes in the photoisomerization of DODCI 206 (1996) 375
- Domcke, W., see Krempel, S. 206 (1996) 63
- Ernest, A.D., see Fewell, M.P. 206 (1996) 257
- Ernest, A.D., see Haydon, S.C. 206 (1996) 245
- Ferrari, L., Diffusion coefficients of ions in lighter gases in an electric field 206 (1996) 9
- Fewell, M.P., S.C. Haydon and A.D. Ernest, Identification of slowly diffusing metastable states of the nitrogen molecule 206 (1996) 257
- Fewell, M.P., see Haydon, S.C. 206 (1996) 245
- Field, C.N., J.C. Green, A.G.J. Moody and M.R.F. Siggel, A photoelectron study of the electronic structure of  $(\eta\text{-C}_6\text{H}_6)\text{Cr}(\text{CO})_3$  and  $(\eta\text{-C}_5\text{H}_5)\text{Mn}(\text{CO})_3$  using variable photon energy 206 (1996) 211

- Galasso, V., Theoretical study of the low-lying excited states of cyclopropane and annelated derivatives 206 (1996) 289
- Garcia-Moreno, I., see Costela, A. 206 (1996) 383
- Gole, J.L., see Stephens, J.M. 206 (1996) 173
- Graener, H., see Hofmann, M. 206 (1996) 129
- Green, J.C., see Field, C.N. 206 (1996) 211
- Gudipati, M.S., Erratum to "Schumann-Runge bands of O<sub>2</sub> in Ar, Kr and Xe matrices revisited: potential curves of the B<sup>3</sup>Σ<sub>u</sub><sup>-</sup> state" [Chem. Phys. 201 (1995) 451-462] 206 (1996) 269
- Guilleme, J., see San Fabián, J. 206 (1996) 325
- Haydon, S.C., M.P. Fewell, A.D. Ernest and M.J. Baldwin, Diffusion coefficients of two metastable states of the nitrogen molecule 206 (1996) 245
- Haydon, S.C., see Fewell, M.P. 206 (1996) 257
- Hofmann, M. and H. Graener, Time resolved incoherent anti-Stokes Raman spectroscopy of dichloromethane 206 (1996) 129
- Karabunarliev, S., see Zhang, J. 206 (1996) 339
- Krempf, S., W. Domcke and M. Winterstetter, Real-time path-integral approach for general two-state multi-mode vibronic-coupling models 206 (1996) 63
- Legay, F. and N. Legay-Sommaire, Cooperative two-phonon absorption in solid α-nitrogen in the 4600-4700 cm<sup>-1</sup> region 206 (1996) 363
- Legay-Sommaire, N., see Legay, F. 206 (1996) 363
- Lehner, O., see Dhuicq, D. 206 (1996) 139
- Linder, F., see Dhuicq, D. 206 (1996) 139
- Locht, R., see Momigny, J. 206 (1996) 225
- Löhmannsröben, H.-G., see Schael, F. 206 (1996) 193
- Luque, J. and D.R. Crosley, Predissociation rates in the B<sup>2</sup>Σ<sup>-</sup> state of CH 206 (1996) 185
- Malagoli, M. and W. Thiel, A semiempirical approach to nonlinear optical properties of large molecules at the MNDO and MNDO/d level 206 (1996) 73
- McNaughton, D., E.G. Robertson and F. Shanks, Vibrational and vibration-rotational spectroscopy of CBrClF<sub>2</sub> (Halon-1211) 206 (1996) 161
- Moliner, V., J. Andrés, A. Arnau, E. Silla and I. Tuñón, Rotational constants and dipole moments of interstellar polyynes: a comparative MP2 and density functional (BP86) study 206 (1996) 57
- Momigny, J. and R. Loch, The appearance of CH<sub>3</sub><sup>+</sup> ions from methyl halides by non-resonant photoionization. A translational energy surprisal analysis. Part I. CH<sub>3</sub>F 206 (1996) 225
- Moody, A.G.J., see Field, C.N. 206 (1996) 211
- Nagaoka, S.-i. and U. Nagashima, Effects of node of wave function upon excited-state intramolecular proton transfer of hydroxyanthraquinones and aminoanthraquinones 206 (1996) 353
- Nagashima, U., see Nagaoka, S.-i. 206 (1996) 353
- Nakashima, K., see Tokeshi, M. 206 (1996) 237
- Nordholm, S., see Bolton, K. 206 (1996) 103
- Ogawa, T., see Tokeshi, M. 206 (1996) 237

- Resende, S.M. and W.B. De Almeida, A theoretical study of tunneling in the (HCCH)<sub>2</sub> complex 206 (1996) 1
- Robertson, E.G., see McNaughton, D. 206 (1996) 161
- Røeggen, I., see Wind, P. 206 (1996) 307
- San Fabián, J. and J. Guilleme, Vicinal fluorine-proton coupling constants. Ab initio calculations of angular dependence and substituent effects 206 (1996) 325
- Schael, F. and H.-G. Löhmannsröben, The deactivation of singlet excited all-trans-1,6-diphenylhexa-1,3,5-triene by intermolecular charge transfer processes. 1. Mechanisms of fluorescence quenching and of triplet and cation formation 206 (1996) 193
- Shanks, F., see McNaughton, D. 206 (1996) 161
- Sidis, V., see Dhuicq, D. 206 (1996) 139
- Siggel, M.R.F., see Field, C.N. 206 (1996) 211
- Silla, E., see Moliner, V. 206 (1996) 57
- Sohlberg, K. and K. Szalewicz, Dynamical coupling of the diatom vibrational motions in collisions of N<sub>2</sub> with N<sub>2</sub><sup>+</sup> 206 (1996) 87
- Stephens, J.M. and J.L. Gole, Controlled formation of state selected SiO metastables using a new pyrolysis source 206 (1996) 173
- Szalewicz, K., see Sohlberg, K. 206 (1996) 87
- Thiel, W., see Malagoli, M. 206 (1996) 73
- Tocho, J.O., see Di Paolo, R.E. 206 (1996) 375
- Tokeshi, M., K. Nakashima and T. Ogawa, Dissociative excitation of aliphatic hydrocarbons (C<sub>2</sub>H<sub>2n</sub>: n = 1, 2, 3) by fast argon ion impact: Rovibrational distribution of CH(A<sup>2</sup>Δ) 206 (1996) 237
- Tuñón, I., see Moliner, V. 206 (1996) 57
- Wang, J.-H., H.-C. Chang and Y.-T. Chen, Theoretical study of isomeric structures and low-lying electronic states of the vinyl radical C<sub>2</sub>H<sub>3</sub> 206 (1996) 43
- Wang, Y. and C. Deng, The correlation-function potential-harmonic and generalized Laguerre function calculation on the <sup>1</sup>S states of the helium atom 206 (1996) 279
- Wind, P. and I. Røeggen, Energy expansion in the extended geminal model 206 (1996) 307
- Winterstetter, M., see Krempel, S. 206 (1996) 63
- Zhang, C.-T. and K.-C. Chou, Beat motion in DNA double helix and a mechanism of energy exchange between its two strands with microwave frequency 206 (1996) 271
- Zhang, J., S. Karabunarliev and M. Baumgarten, The ground state spin multiplicity of Schlenk-type biradicals and the influence of additional linkage to ladder type structures 206 (1996) 339

6

6

1

## Subject index to volume 206

### Methods

#### Theoretical

##### *Group theory and algebras*

- A theoretical study of tunneling in the  $(\text{HCCH})_2$  complex, S.M. Resende and W.B. De Almeida 206 (1996) 1

##### *Classical mechanics*

- Beat motion in DNA double helix and a mechanism of energy exchange between its two strands with microwave frequency, C.-T. Zhang and K.-C. Chou 206 (1996) 271

##### *Many body and quasiparticle approaches*

- The correlation-function potential-harmonic and generalized Laguerre function calculation on the  $^1\text{S}$  states of the helium atom, Y. Wang and C. Deng 206 (1996) 279
- Theoretical study of the low-lying excited states of cyclopropane and annelated derivatives, V. Galasso 206 (1996) 289

##### *Statistical mechanics of stationary states*

- A prediction for the thermal conductivity coefficient of liquids along the saturation line, J. Amorós 206 (1996) 301

##### *Non-equilibrium thermodynamic and hydrodynamic theories*

- Diffusion coefficients of ions in lighter gases in an electric field, L. Ferrari 206 (1996) 9

##### *Ab initio schemes for stationary properties*

- A theoretical study of tunneling in the  $(\text{HCCH})_2$  complex, S.M. Resende and W.B. De Almeida 206 (1996) 1
- The structure of  $\text{Li}^-$  and  $\text{K}^-$ , C.W. Bauschlicher Jr. 206 (1996) 35
- Theoretical study of isomeric structures and low-lying electronic states of the vinyl radical  $\text{C}_2\text{H}_3$ , J.-H. Wang, H.-C. Chang and Y.-T. Chen 206 (1996) 43
- Rotational constants and dipole moments of interstellar polyynes: a comparative MP2 and density functional (BP86) study, V. Moliner, J. Andrés, A. Arnau, E. Silla and I. Tuñón 206 (1996) 57
- Energy expansion in the extended geminal model, P. Wind and I. Røeggen 206 (1996) 307

*Computational and simulation methods*

- Theoretical study of isomeric structures and low-lying electronic states of the vinyl radical  $C_2H_3$ , J.-H. Wang, H.-C. Chang and Y.-T. Chen 206 (1996) 43
- Rotational constants and dipole moments of interstellar polyynes: a comparative MP2 and density functional (BP86) study, V. Moliner, J. Andrés, A. Arnau, E. Silla and I. Tuñón 206 (1996) 57
- Real-time path-integral approach for general two-state multi-mode vibronic-coupling models, S. Kreml, W. Domcke and M. Winterstetter 206 (1996) 63
- A semiempirical approach to nonlinear optical properties of large molecules at the MNDO and MNDO/d level, M. Malagoli and W. Thiel 206 (1996) 73
- The correlation-function potential-harmonic and generalized Laguerre function calculation on the  $^1S$  states of the helium atom, Y. Wang and C. Deng 206 (1996) 279
- Vicinal fluorine-proton coupling constants. Ab initio calculations of angular dependence and substituent effects, J. San Fabián and J. Guilleme 206 (1996) 325
- The ground state spin multiplicity of Schlenk-type biradicals and the influence of additional linkage to ladder type structures, J. Zhang, S. Karabunarliev and M. Baumgarten 206 (1996) 339

*Molecular dynamics and scattering theory*

- Dynamical coupling of the diatom vibrational motions in collisions of  $N_2$  with  $N_2^+$ , K. Sohlberg and K. Szalewicz 206 (1996) 87
- Classical trajectory study of collision induced intramolecular energy transfer in trans-stilbene, K. Bolton and S. Nordholm 206 (1996) 103
- Time resolved incoherent anti-Stokes Raman spectroscopy of dichloromethane, M. Hofmann and H. Graener 206 (1996) 129
- Angular and energy analysis of  $HeH^+$  products from the charge exchange excitation reaction  $He^+ + H_2 \rightarrow HeH^+ + H^+$ , D. Dhuicq, O. Lehner, F. Linder and V. Sidis 206 (1996) 139
- Effects of node of wave function upon excited-state intramolecular proton transfer of hydroxyanthraquinones and aminoanthraquinones, S.-i. Nagaoka and U. Nagashima 206 (1996) 353

**Experimental***Infrared spectroscopy*

- Vibrational and vibration-rotational spectroscopy of  $CBrClF_2$  (Halon-1211), D. McNaughton, E.G. Robertson and F. Shanks 206 (1996) 161
- Cooperative two-phonon absorption in solid  $\alpha$ -nitrogen in the 4600–4700  $cm^{-1}$  region, F. Legay and N. Legay-Sommaire 206 (1996) 363

*Visible and UV spectroscopy*

- Controlled formation of state selected SiO metastables using a new pyrolysis source, J.M. Stephens and J.L. Gole 206 (1996) 173
- Predissociation rates in the  $B^2\Sigma^-$  state of CH, J. Luque and D.R. Crosley 206 (1996) 185

*Fluorescence spectroscopy*

- Predissociation rates in the  $B^2\Sigma^-$  state of CH, J. Luque and D.R. Crosley 206 (1996) 185
- The deactivation of singlet excited all-trans-1,6-diphenylhexa-1,3,5-triene by intermolecular charge transfer processes. 1. Mechanisms of fluorescence quenching and of triplet and cation formation, F. Schael and H.-G. Löhmannsröben 206 (1996) 193

- Polarization anisotropy applied to the determination of structural changes in the photoisomerization of DODCI, R.E. Di Paolo and J.O. Tocho 206 (1996) 375
- Photoelectron and Auger spectroscopy*
- A photoelectron study of the electronic structure of  $(\eta\text{-C}_6\text{H}_6)\text{Cr}(\text{CO})_3$  and  $(\eta\text{-C}_5\text{H}_5)\text{Mn}(\text{CO})_3$  using variable photon energy, C.N. Field, J.C. Green, A.G.J. Moody and M.R.F. Siggel 206 (1996) 211
- Laser methods*
- Phase-conjugate reflection by degenerate four-wave mixing in 2-(2'-hydroxyphenyl)benzimidazole dye solutions: solvent effects, A. Costela and I. Garcia-Moreno 206 (1996) 383
- Picosecond spectroscopy*
- Time resolved incoherent anti-Stokes Raman spectroscopy of dichloromethane, M. Hoffmann and H. Graener 206 (1996) 129
- Synchrotron spectroscopies*
- The appearance of  $\text{CH}_3^+$  ions from methyl halides by non-resonant photoionization. A translational energy surprisal analysis. Part I.  $\text{CH}_3\text{F}$ , J. Momigny and R. Loch 206 (1996) 225
- Atomic and molecular beam techniques*
- Angular and energy analysis of  $\text{HeH}^+$  products from the charge exchange excitation reaction  $\text{He}^+ + \text{H}_2 \rightarrow \text{HeH}^+ + \text{H}^+$ , D. Dhucq, O. Lehner, F. Linder and V. Sidis 206 (1996) 139
- Dissociative excitation of aliphatic hydrocarbons ( $\text{C}_2\text{H}_{2n}$ ;  $n = 1, 2, 3$ ) by fast argon ion impact: Rovibrational distribution of  $\text{CH}(\text{A}^2\Delta)$ , M. Tokeshi, K. Nakashima and T. Ogawa 206 (1996) 237
- Time-resolved experiments*
- The deactivation of singlet excited all-trans-1,6-diphenylhexa-1,3,5-triene by intermolecular charge transfer processes. 1. Mechanisms of fluorescence quenching and of triplet and cation formation, F. Schael and H.-G. Löhmannsröben 206 (1996) 193
- Diffusion coefficients of two metastable states of the nitrogen molecule, S.C. Haydon, M.P. Fewell, A.D. Ernest and M.J. Baldwin 206 (1996) 245
- Mass spectrometry*
- The appearance of  $\text{CH}_3^+$  ions from methyl halides by non-resonant photoionization. A translational energy surprisal analysis. Part I.  $\text{CH}_3\text{F}$ , J. Momigny and R. Loch 206 (1996) 225
- Light scattering*
- Phase-conjugate reflection by degenerate four-wave mixing in 2-(2'-hydroxyphenyl)benzimidazole dye solutions: solvent effects, A. Costela and I. Garcia-Moreno 206 (1996) 383
- Measurement of macroscopic variables*
- Diffusion coefficients of two metastable states of the nitrogen molecule, S.C. Haydon, M.P. Fewell, A.D. Ernest and M.J. Baldwin 206 (1996) 245
- Identification of slowly diffusing metastable states of the nitrogen molecule, M.P. Fewell, S.C. Haydon and A.D. Ernest 206 (1996) 257



## Objects

### Bulk systems

#### Gases

- Diffusion coefficients of ions in lighter gases in an electric field, L. Ferrari 206 (1996) 9
- Controlled formation of state selected SiO metastables using a new pyrolysis source, J.M. Stephens and J.L. Gole 206 (1996) 173
- The appearance of  $\text{CH}_3^+$  ions from methyl halides by non-resonant photoionization. A translational energy surprisal analysis. Part I.  $\text{CH}_3\text{F}$ , J. Momigny and R. Loch 206 (1996) 225

#### Supersonic beams

- Vibrational and vibration-rotational spectroscopy of  $\text{CBrClF}_2$  (Halon-1211), D. McNaughton, E.G. Robertson and F. Shanks 206 (1996) 161

#### Liquids neat

- Time resolved incoherent anti-Stokes Raman spectroscopy of dichloromethane, M. Hofmann and H. Graener 206 (1996) 129
- A prediction for the thermal conductivity coefficient of liquids along the saturation line, J. Amorós 206 (1996) 301

#### Liquid mixtures and solutions

- Phase-conjugate reflection by degenerate four-wave mixing in 2-(2'-hydroxyphenyl)benzimidazole dye solutions: solvent effects, A. Costela and I. Garcia-Moreno 206 (1996) 383

#### Crystals

- Cooperative two-phonon absorption in solid  $\alpha$ -nitrogen in the  $4600\text{--}4700\text{ cm}^{-1}$  region, F. Legay and N. Legay-Sommaire 206 (1996) 363

#### Glasses

- Beat motion in DNA double helix and a mechanism of energy exchange between its two strands with microwave frequency, C.-T. Zhang and K.-C. Chou 206 (1996) 271

### Microscopic systems

#### Atoms

- The correlation-function potential-harmonic and generalized Laguerre function calculation on the  $^1\text{S}$  states of the helium atom, Y. Wang and C. Deng 206 (1996) 279

#### Molecules (neutral and ionic)

- Real-time path-integral approach for general two-state multi-mode vibronic-coupling models, S. Kreml, W. Domcke and M. Winterstetter 206 (1996) 63
- Angular and energy analysis of  $\text{HeH}^+$  products from the charge exchange excitation reaction  $\text{He}^+ + \text{H}_2 \rightarrow \text{HeH}^+ + \text{H}^+$ , D. Dhucq, O. Lehner, F. Linder and V. Sidis 206 (1996) 139
- A photoelectron study of the electronic structure of  $(\eta\text{-C}_6\text{H}_6)\text{Cr}(\text{CO})_3$  and  $(\eta\text{-C}_5\text{H}_5)\text{Mn}(\text{CO})_3$  using variable photon energy, C.N. Field, J.C. Green, A.G.J. Moody and M.R.F. Siggel 206 (1996) 211



- Polarization anisotropy applied to the determination of structural changes in the photoisomerization of DODCl, R.E. Di Paolo and J.O. Tocho 206 (1996) 375
- diatomic*
- Dynamical coupling of the diatom vibrational motions in collisions of  $N_2$  with  $N_2^+$ , K. Sohlberg and K. Szalewicz 206 (1996) 87
- Controlled formation of state selected SiO metastables using a new pyrolysis source, J.M. Stephens and J.L. Gole 206 (1996) 173
- Predissociation rates in the  $B^2\Sigma^-$  state of CH, J. Luque and D.R. Crosley 206 (1996) 185
- Diffusion coefficients of two metastable states of the nitrogen molecule, S.C. Haydon, M.P. Fewell, A.D. Ernest and M.J. Baldwin 206 (1996) 245
- Identification of slowly diffusing metastable states of the nitrogen molecule, M.P. Fewell, S.C. Haydon and A.D. Ernest 206 (1996) 257
- small polyatomics*
- The structure of  $Li_7^-$  and  $K_7^-$ , C.W. Bauschlicher Jr. 206 (1996) 35
- Theoretical study of isomeric structures and low-lying electronic states of the vinyl radical  $C_2H_3$ , J.-H. Wang, H.-C. Chang and Y.-T. Chen 206 (1996) 43
- Rotational constants and dipole moments of interstellar polyynes: a comparative MP2 and density functional (BP86) study, V. Moliner, J. Andrés, A. Arnau, E. Silla and I. Tuñón 206 (1996) 57
- Time resolved incoherent anti-Stokes Raman spectroscopy of dichloromethane, M. Hofmann and H. Graener 206 (1996) 129
- Vibrational and vibration-rotational spectroscopy of  $CBrClF_2$  (Halon-1211), D. McNaughton, E.G. Robertson and F. Shanks 206 (1996) 161
- The appearance of  $CH_3^+$  ions from methyl halides by non-resonant photoionization. A translational energy surprisal analysis. Part I.  $CH_3F$ , J. Momigny and R. Loch 206 (1996) 225
- Dissociative excitation of aliphatic hydrocarbons ( $C_2H_{2n}$ :  $n = 1, 2, 3$ ) by fast argon ion impact: Rovibrational distribution of  $CH(A^2\Delta)$ , M. Tokeshi, K. Nakashima and T. Ogawa 206 (1996) 237
- Theoretical study of the low-lying excited states of cyclopropane and annelated derivatives, V. Galasso 206 (1996) 289
- Vicinal fluorine-proton coupling constants. Ab initio calculations of angular dependence and substituent effects, J. San Fabián and J. Guilleme 206 (1996) 325
- aromatics*
- Classical trajectory study of collision induced intramolecular energy transfer in trans-stilbene, K. Bolton and S. Nordholm 206 (1996) 103
- The ground state spin multiplicity of Schlenk-type biradicals and the influence of additional linkage to ladder type structures, J. Zhang, S. Karabunarliev and M. Baumgarten 206 (1996) 339
- Effects of node of wave function upon excited-state intramolecular proton transfer of hydroxyanthraquinones and aminoanthraquinones, S.-i. Nagaoka and U. Nagashima 206 (1996) 353
- other large*
- A photoelectron study of the electronic structure of  $(\eta-C_6H_6)Cr(CO)_3$  and  $(\eta-C_5H_5)Mn(CO)_3$  using variable photon energy, C.N. Field, J.C. Green, A.G.J. Moody and M.R.F. Siggel 206 (1996) 211

*Molecular aggregates**-dimers*

- A theoretical study of tunneling in the (HCCH)<sub>2</sub> complex, S.M. Resende and W.B. De Almeida 206 (1996) 1
- Identification of slowly diffusing metastable states of the nitrogen molecule, M.P. Fewell, S.C. Haydon and A.D. Ernest 206 (1996) 257

*-van der Waals molecules*

- Energy expansion in the extended geminal model, P. Wind and I. Røeggen 206 (1996) 307

*-clusters*

- The structure of Li<sub>7</sub><sup>-</sup> and K<sub>7</sub><sup>-</sup>, C.W. Bauschlicher Jr. 206 (1996) 35

*-complexes*

- The deactivation of singlet excited all-trans-1,6-diphenylhexa-1,3,5-triene by intermolecular charge transfer processes. 1. Mechanisms of fluorescence quenching and of triplet and cation formation, F. Schael and H.-G. Löhmansröben 206 (1996) 193

*Free radicals (including hydronium and muonium)*

- Theoretical study of isomeric structures and low-lying electronic states of the vinyl radical C<sub>2</sub>H<sub>3</sub>, J.-H. Wang, H.-C. Chang and Y.-T. Chen 206 (1996) 43

*Ions and charge carriers*

- Diffusion coefficients of ions in lighter gases in an electric field, L. Ferrari 206 (1996) 9

**Phenomena***Molecular structure*

- The structure of Li<sub>7</sub><sup>-</sup> and K<sub>7</sub><sup>-</sup>, C.W. Bauschlicher Jr. 206 (1996) 35
- Rotational constants and dipole moments of interstellar polyynes: a comparative MP2 and density functional (BP86) study, V. Moliner, J. Andrés, A. Arnau, E. Silla and I. Tuñón 206 (1996) 57
- The ground state spin multiplicity of Schlenk-type biradicals and the influence of additional linkage to ladder type structures, J. Zhang, S. Karabunarliev and M. Baumgarten 206 (1996) 339

*Vibrations and rotations of molecules*

- A theoretical study of tunneling in the (HCCH)<sub>2</sub> complex, S.M. Resende and W.B. De Almeida 206 (1996) 1
- Rotational constants and dipole moments of interstellar polyynes: a comparative MP2 and density functional (BP86) study, V. Moliner, J. Andrés, A. Arnau, E. Silla and I. Tuñón 206 (1996) 57
- Time resolved incoherent anti-Stokes Raman spectroscopy of dichloromethane, M. Hofmann and H. Graener 206 (1996) 129
- Vibrational and vibration-rotational spectroscopy of CBrClF<sub>2</sub> (Halon-1211), D. McNaughton, E.G. Robertson and F. Shanks 206 (1996) 161
- Dissociative excitation of aliphatic hydrocarbons (C<sub>2</sub>H<sub>2n</sub>; n = 1, 2, 3) by fast argon ion impact: Rovibrational distribution of CH(A<sup>2</sup>Δ), M. Tokeshi, K. Nakashima and T. Ogawa 206 (1996) 237

- Beat motion in DNA double helix and a mechanism of energy exchange between its two strands with microwave frequency, C.-T. Zhang and K.-C. Chou 206 (1996) 271
- Electronic structure and states*
- The structure of  $\text{Li}^-$  and  $\text{K}^-$ , C.W. Bauschlicher Jr. 206 (1996) 35
- Theoretical study of isomeric structures and low-lying electronic states of the vinyl radical  $\text{C}_2\text{H}_3$ , J.-H. Wang, H.-C. Chang and Y.-T. Chen 206 (1996) 43
- Predissociation rates in the  $\text{B}^2\Sigma^-$  state of CH, J. Luque and D.R. Crosley 206 (1996) 185
- A photoelectron study of the electronic structure of  $(\eta\text{-C}_6\text{H}_6)\text{Cr}(\text{CO})_3$  and  $(\eta\text{-C}_5\text{H}_5)\text{Mn}(\text{CO})_3$  using variable photon energy, C.N. Field, J.C. Green, A.G.J. Moody and M.R.F. Siggel 206 (1996) 211
- The correlation-function potential-harmonic and generalized Laguerre function calculation on the  $^1\text{S}$  states of the helium atom, Y. Wang and C. Deng 206 (1996) 279
- Theoretical study of the low-lying excited states of cyclopropane and annelated derivatives, V. Galasso 206 (1996) 289
- Electric and magnetic properties*
- Diffusion coefficients of ions in lighter gases in an electric field, L. Ferrari 206 (1996) 9
- The ground state spin multiplicity of Schlenk-type biradicals and the influence of additional linkage to ladder type structures, J. Zhang, S. Karabunarliev and M. Baumgarten 206 (1996) 339
- Spin splittings*
- Vicinal fluorine-proton coupling constants. Ab initio calculations of angular dependence and substituent effects, J. San Fabián and J. Guilleme 206 (1996) 325
- The ground state spin multiplicity of Schlenk-type biradicals and the influence of additional linkage to ladder type structures, J. Zhang, S. Karabunarliev and M. Baumgarten 206 (1996) 339
- Molecular interactions*
- Energy expansion in the extended geminal model, P. Wind and I. Røeggen 206 (1996) 307
- Cooperative two-phonon absorption in solid  $\alpha$ -nitrogen in the  $4600\text{--}4700\text{ cm}^{-1}$  region, F. Legay and N. Legay-Sommaire 206 (1996) 363
- Spectral bandshapes and intensities*
- Vibrational and vibration-rotational spectroscopy of  $\text{CBrClF}_2$  (Halon-1211), D. McNaughton, E.G. Robertson and F. Shanks 206 (1996) 161
- Predissociation rates in the  $\text{B}^2\Sigma^-$  state of CH, J. Luque and D.R. Crosley 206 (1996) 185
- Cooperative two-phonon absorption in solid  $\alpha$ -nitrogen in the  $4600\text{--}4700\text{ cm}^{-1}$  region, F. Legay and N. Legay-Sommaire 206 (1996) 363
- Coupling of electronic and nuclear motion*
- Angular and energy analysis of  $\text{HeH}^+$  products from the charge exchange excitation reaction  $\text{He}^+ + \text{H}_2 \rightarrow \text{HeH}^+ + \text{H}^+$ , D. Dhucq, O. Lehner, F. Linder and V. Sidis 206 (1996) 139
- Energy transfer processes*
- Dynamical coupling of the diatom vibrational motions in collisions of  $\text{N}_2$  with  $\text{N}_2^+$ , K. Sohlberg and K. Szalewicz 206 (1996) 87
- Classical trajectory study of collision induced intramolecular energy transfer in trans-stilbene, K. Bolton and S. Nordholm 206 (1996) 103

- Controlled formation of state selected SiO metastables using a new pyrolysis source, J.M. Stephens and J.L. Gole 206 (1996) 173
- Phase-conjugate reflection by degenerate four-wave mixing in 2-(2'-hydroxyphenyl)benzimidazole dye solutions: solvent effects, A. Costela and I. Garcia-Moreno 206 (1996) 383
- Molecular photophysical processes*
- Polarization anisotropy applied to the determination of structural changes in the photoisomerization of DODCI, R.E. Di Paolo and J.O. Tocho 206 (1996) 375
- Intramolecular dynamics*
- Real-time path-integral approach for general two-state multi-mode vibronic-coupling models, S. Krempel, W. Domcke and M. Winterstetter 206 (1996) 63
- Classical trajectory study of collision induced intramolecular energy transfer in trans-stilbene, K. Bolton and S. Nordholm 206 (1996) 103
- The appearance of  $\text{CH}_3^+$  ions from methyl halides by non-resonant photoionization. A translational energy surprisal analysis. Part I.  $\text{CH}_3\text{F}$ , J. Momigny and R. Locht 206 (1996) 225
- vibrational energy redistribution (including vibrational dissociation)*
- Identification of slowly diffusing metastable states of the nitrogen molecule, M.P. Fewell, S.C. Haydon and A.D. Ernest 206 (1996) 257
- Luminescence spectra, yields and lifetimes*
- The deactivation of singlet excited all-trans-1,6-diphenylhexa-1,3,5-triene by intermolecular charge transfer processes. 1. Mechanisms of fluorescence quenching and of triplet and cation formation, F. Schael and H.-G. Löhmannsröben 206 (1996) 193
- Non-linear responses (including optical)*
- A semiempirical approach to nonlinear optical properties of large molecules at the MNDO and MNDO/d level, M. Malagoli and W. Thiel 206 (1996) 73
- Phase-conjugate reflection by degenerate four-wave mixing in 2-(2'-hydroxyphenyl)benzimidazole dye solutions: solvent effects, A. Costela and I. Garcia-Moreno 206 (1996) 383
- Reactions (including dissociation)*
- Classical trajectory study of collision induced intramolecular energy transfer in trans-stilbene, K. Bolton and S. Nordholm 206 (1996) 103
- gas phase*
- Angular and energy analysis of  $\text{HeH}^+$  products from the charge exchange excitation reaction  $\text{He}^+ + \text{H}_2 \rightarrow \text{HeH}^+ + \text{H}^+$ , D. Dhucq, O. Lehner, F. Linder and V. Sidis 206 (1996) 139
- Controlled formation of state selected SiO metastables using a new pyrolysis source, J.M. Stephens and J.L. Gole 206 (1996) 173
- Dissociative excitation of aliphatic hydrocarbons ( $\text{C}_2\text{H}_{2n}$ :  $n = 1, 2, 3$ ) by fast argon ion impact: Rovibrational distribution of  $\text{CH}(\text{A}^2\Delta)$ , M. Tokeshi, K. Nakashima and T. Ogawa 206 (1996) 237
- Diffusion coefficients of two metastable states of the nitrogen molecule, S.C. Haydon, M.P. Fewell, A.D. Ernest and M.J. Baldwin 206 (1996) 245
- Identification of slowly diffusing metastable states of the nitrogen molecule, M.P. Fewell, S.C. Haydon and A.D. Ernest 206 (1996) 257

*-photochemical*

- Effects of node of wave function upon excited-state intramolecular proton transfer of hydroxyanthraquinones and aminoanthraquinones, S.-i. Nagaoka and U. Nagashima 206 (1996) 353

*Tunnelling*

- A theoretical study of tunneling in the  $(\text{HCCH})_2$  complex, S.M. Resende and W.B. De Almeida 206 (1996) 1

*Electron transfer*

- The deactivation of singlet excited all-trans-1,6-diphenylhexa-1,3,5-triene by intermolecular charge transfer processes. 1. Mechanisms of fluorescence quenching and of triplet and cation formation, F. Schael and H.-G. Löhmannsröben 206 (1996) 193

*Ionization (including Rydberg states)*

- A photoelectron study of the electronic structure of  $(\eta\text{-C}_6\text{H}_6)\text{Cr}(\text{CO})_3$  and  $(\eta\text{-C}_5\text{H}_5)\text{Mn}(\text{CO})_3$  using variable photon energy, C.N. Field, J.C. Green, A.G.J. Moody and M.R.F. Siggel 206 (1996) 211

*Molecular motion (including diffusive)*

- Diffusion coefficients of two metastable states of the nitrogen molecule, S.C. Haydon, M.P. Fewell, A.D. Ernest and M.J. Baldwin 206 (1996) 245
- Polarization anisotropy applied to the determination of structural changes in the photoisomerization of DODCI, R.E. Di Paolo and J.O. Tocho 206 (1996) 375

*Isotopic effects*

- Vibrational and vibration-rotational spectroscopy of  $\text{CBrClF}_2$  (Halon-1211), D. McNaughton, E.G. Robertson and F. Shanks 206 (1996) 161

*Thermodynamic and transport properties*

- Diffusion coefficients of ions in lighter gases in an electric field, L. Ferrari 206 (1996) 9
- A prediction for the thermal conductivity coefficient of liquids along the saturation line, J. Amorós 206 (1996) 301